LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121621\
Data File : BF126207.D
Acq On : 16 Dec 2021 12:25
Operator : JU/CG
Sample : PB141409BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PB141409BL

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126207.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.140 | 3 | 9 | 16 | rVB | 81892 | 109685 | 1.82% | 0.269% |
| 2 | 5.046 | 499 | 503 | 510 | rVB | 52791 | 71769 | 1.19% | 0.176% |
| 3 | 5.428 | 562 | 568 | 572 | rBV | 5049622 | 6018966 | 100.00% | 14.750% |
| 4 | 6.440 | 733 | 740 | 743 | rBV | 5058260 | 6014623 | 99.93% | 14.739% |
| 5 | 6.816 | 800 | 804 | 807 | rBV | 1482878 | 1265552 | 21.03% | 3.101% |
| 6 | 7.375 | 893 | 899 | 902 | rBV | 3865560 | 4152185 | 68.99% | 10.175% |
| 7 | 8.098 | 1017 | 1022 | 1025 | rBV | 1862310 | 1823826 | 30.30% | 4.469% |
| 8 | 9.175 | 1199 | 1205 | 1208 | rBV | 5681750 | 6005324 | 99.77% | 14.716% |
| 9 | 9.851 | 1315 | 1320 | 1323 | rBV | 2295678 | 1909358 | 31.72% | 4.679% |
| 10 | 10.639 | 1449 | 1454 | 1457 | rBV | 3438364 | 3396989 | 56.44% | 8.325% |
| 11 | 11.333 | 1568 | 1572 | 1575 | rBV | 2148980 | 1805562 | 30.00% | 4.425% |
| 12 | 12.927 | 1837 | 1843 | 1846 | rBV | 4900806 | 5266100 | 87.49% | 12.905% |
| 13 | 13.969 | 2016 | 2020 | 2023 | rBV | 1337447 | 1254927 | 20.85% | 3.075% |
| 14 | 15.092 | 2207 | 2211 | 2216 | rBV | 86366 | 97682 | 1.62% | 0.239% |
| 15 | 15.410 | 2260 | 2265 | 2270 | rBV | 851961 | 999321 | 16.60% | 2.449% |
| 16 | 15.468 | 2271 | 2275 | 2282 | rVB | 116133 | 149049 | 2.48% | 0.365% |
| 17 | 15.898 | 2343 | 2348 | 2356 | rBV | 88092 | 144601 | 2.40% | 0.354% |
| 18 | 16.398 | 2427 | 2433 | 2440 | rBV2 | 72541 | 135465 | 2.25% | 0.332% |
| 19 | 16.986 | 2526 | 2533 | 2544 | rBV3 | 44952 | 102536 | 1.70% | 0.251% |
| 20 | 17.680 | 2641 | 2651 | 2658 | rBV4 | 29692 | 83309 | 1.38% | 0.204% |

Sum of corrected areas: 40806829

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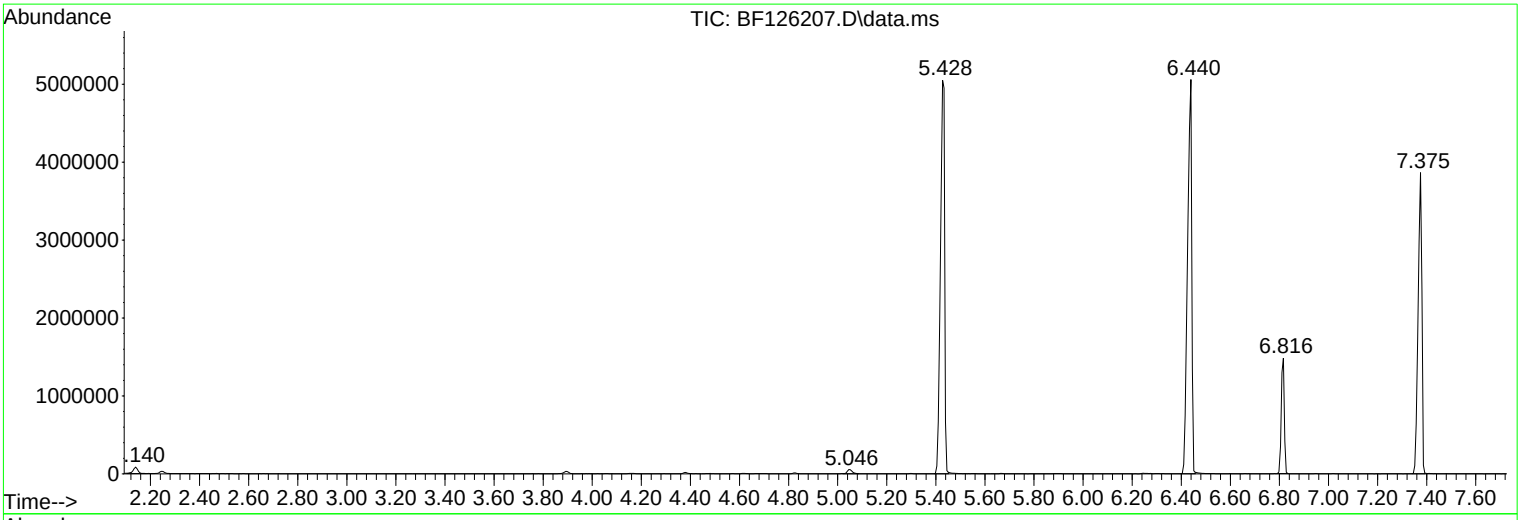
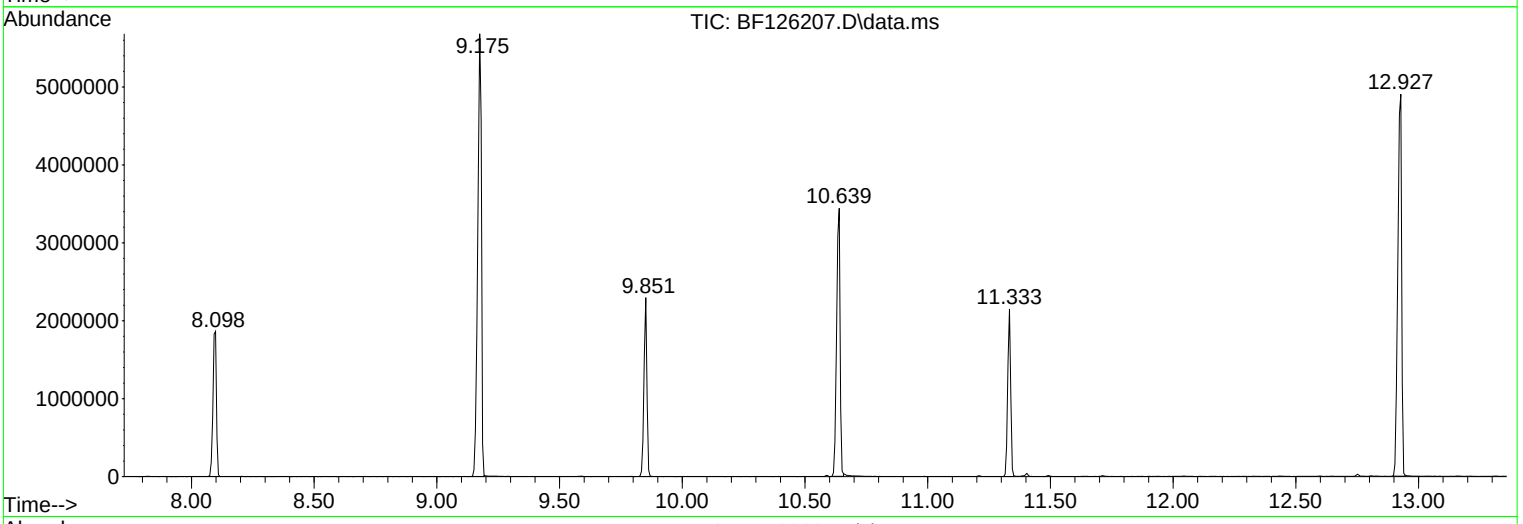
Misc :
ALS Vial : 3 Sample Multiplier: 1

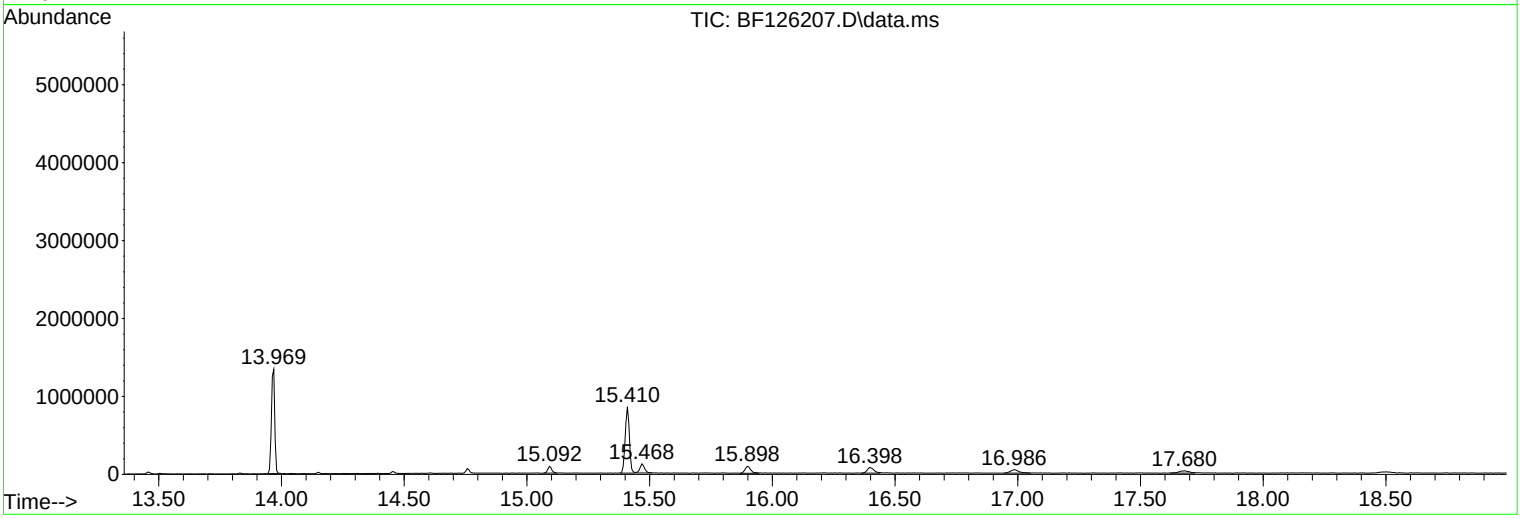
**Instrument :**
BNA_F
**ClientSampleId :**
PB141409BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Data File : BF126207.D
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Sample : PB141409BL
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ALS Vial : 3 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PB141409BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

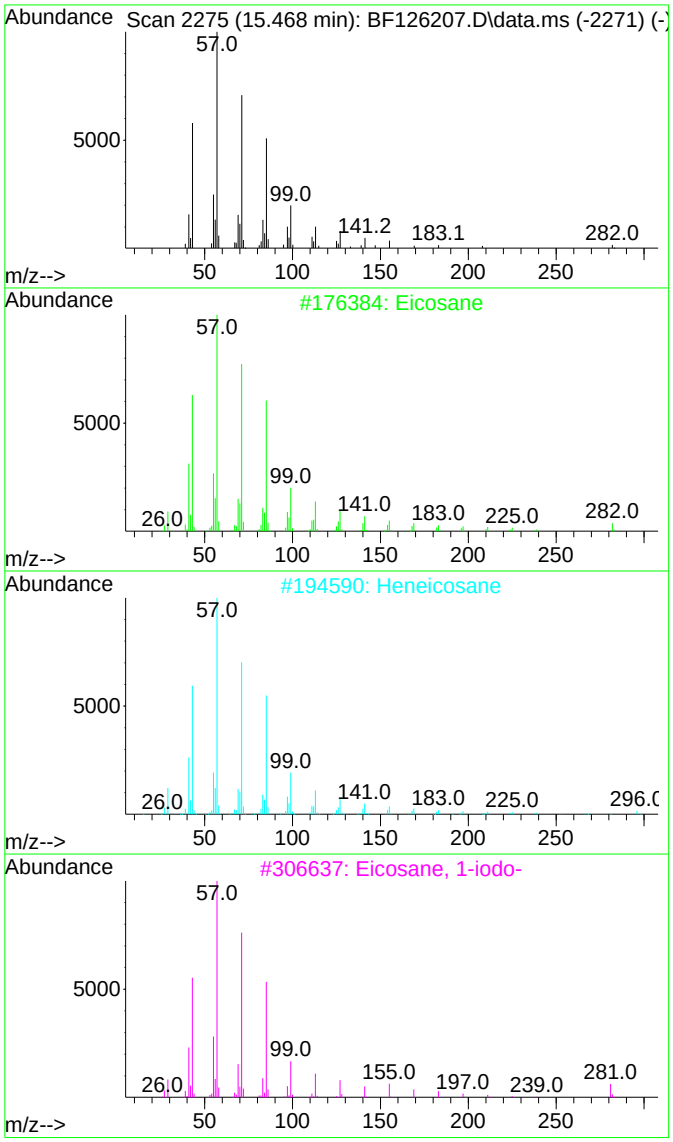
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

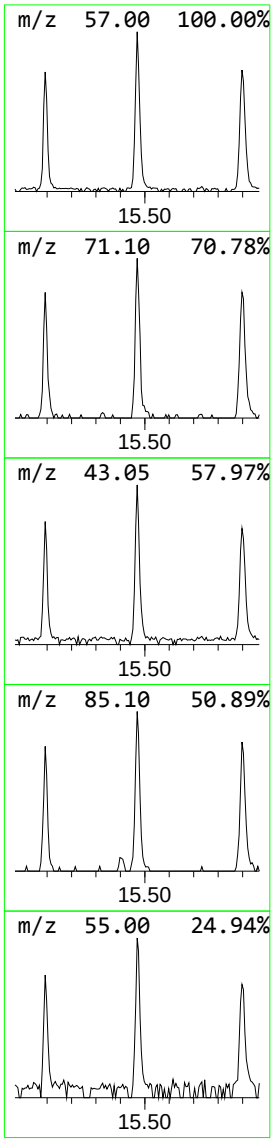
**********

Peak Number 1 Eicosane Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.468 | 2.98 ng | 149049 | Perylene-d12 | 15.410 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 93 |
| 2 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 3 | Eicosane, 1-iodo- | 408 | C20H41I | 1000406-31-8 | 91 |
| 4 | 2-Bromotetradecane | 276 | C14H29Br | 074036-95-6 | 91 |
| 5 | Triacontane | 422 | C30H62 | 000638-68-6 | 90 |



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Sample : PB141409BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PB141409BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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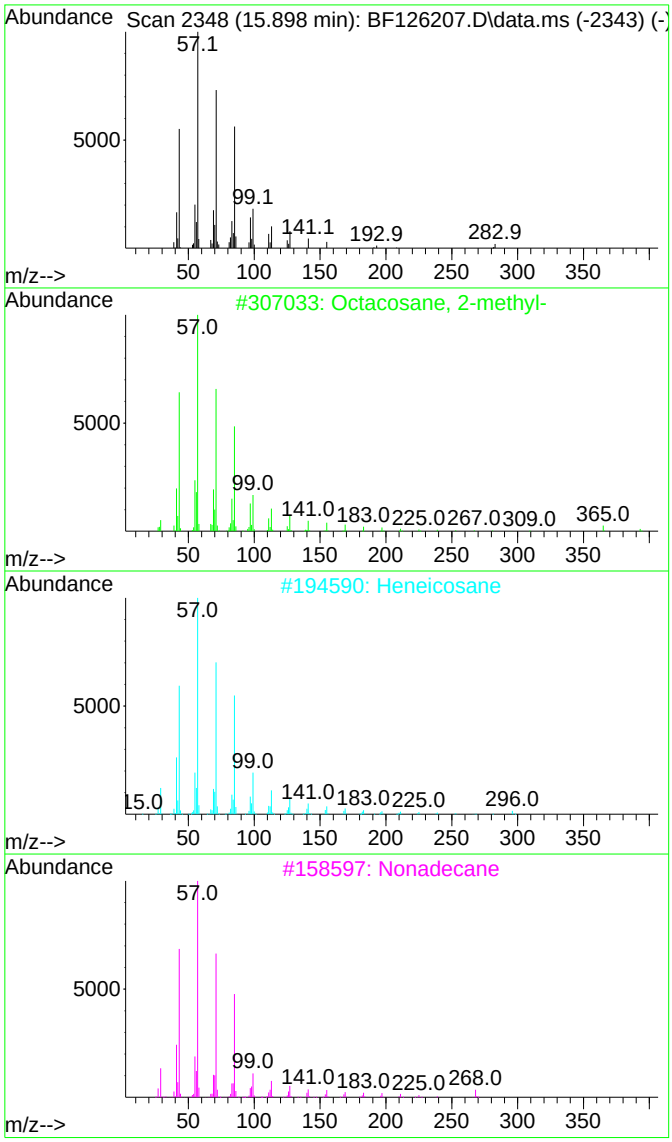
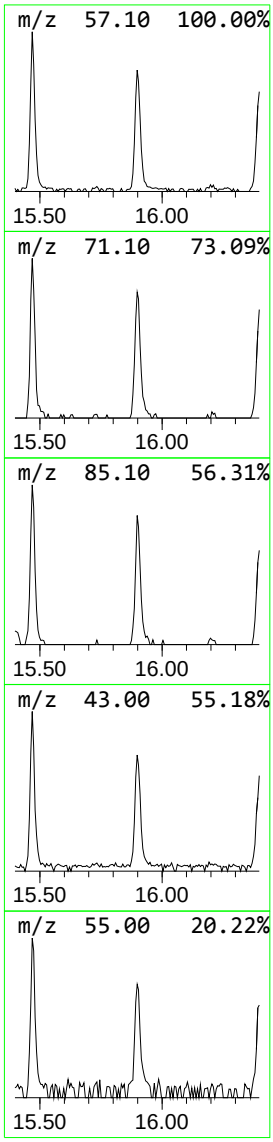
Peak Number 2 Octacosane, 2-methyl- Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.898 | 2.89 ng | 144601 | Perylene-d12 | 15.410 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octacosane, 2-methyl- | 408 | C29H60 | 001560-98-1 | 90 |
| 2 | Heneicosane | 296 | C21H44 | 000629-94-7 | 87 |
| 3 | Nonadecane | 268 | C19H40 | 000629-92-5 | 86 |
| 4 | 2-Bromotetradecane | 276 | C14H29Br | 074036-95-6 | 86 |
| 5 | Octadecane | 254 | C18H38 | 000593-45-3 | 80 |



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Data File : BF126207.D
Acq On : 16 Dec 2021 12:25
Operator : JU/CG
Sample : PB141409BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PB141409BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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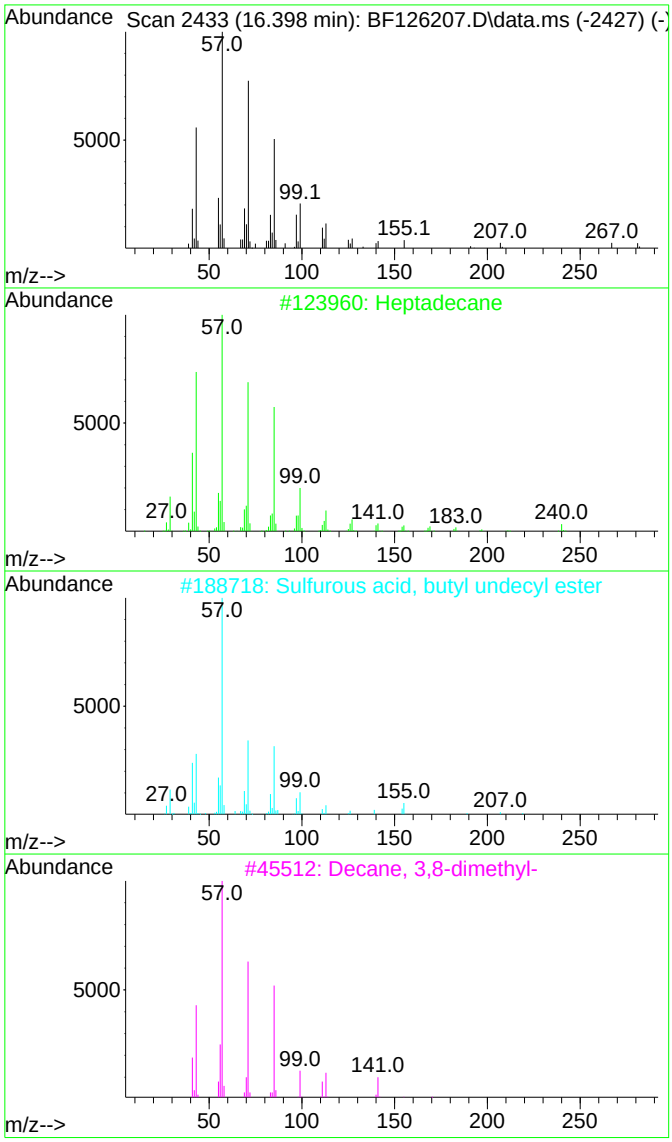
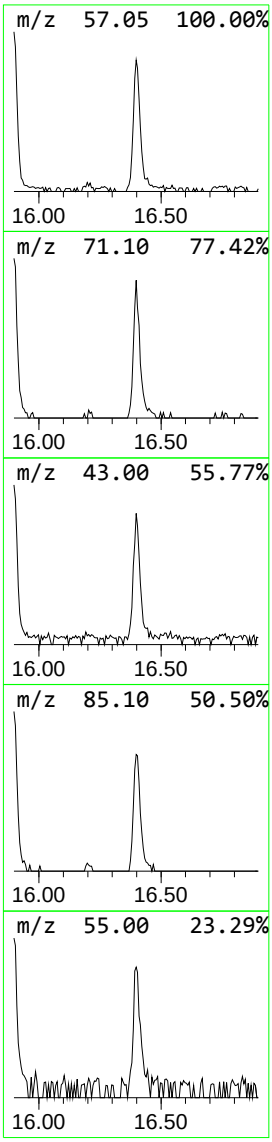
Peak Number 3 Heptadecane Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.398 | 2.71 ng | 135465 | Perylene-d12 | 15.410 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptadecane | 240 | C17H36 | 000629-78-7 | 80 |
| 2 | Sulfurous acid, butyl undecyl ester | 292 | C15H32O3S | 1000309-17-8 | 72 |
| 3 | Decane, 3,8-dimethyl- | 170 | C12H26 | 017312-55-9 | 64 |
| 4 | Sulfurous acid, butyl dodecyl ester | 306 | C16H34O3S | 1000309-17-9 | 58 |
| 5 | Hexadecane, 2,6,10,14-tetramethyl- | 282 | C20H42 | 000638-36-8 | 58 |



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Operator : JU/CG
Sample : PB141409BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PB141409BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
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TIC Library : C:\Database\NIST20.L
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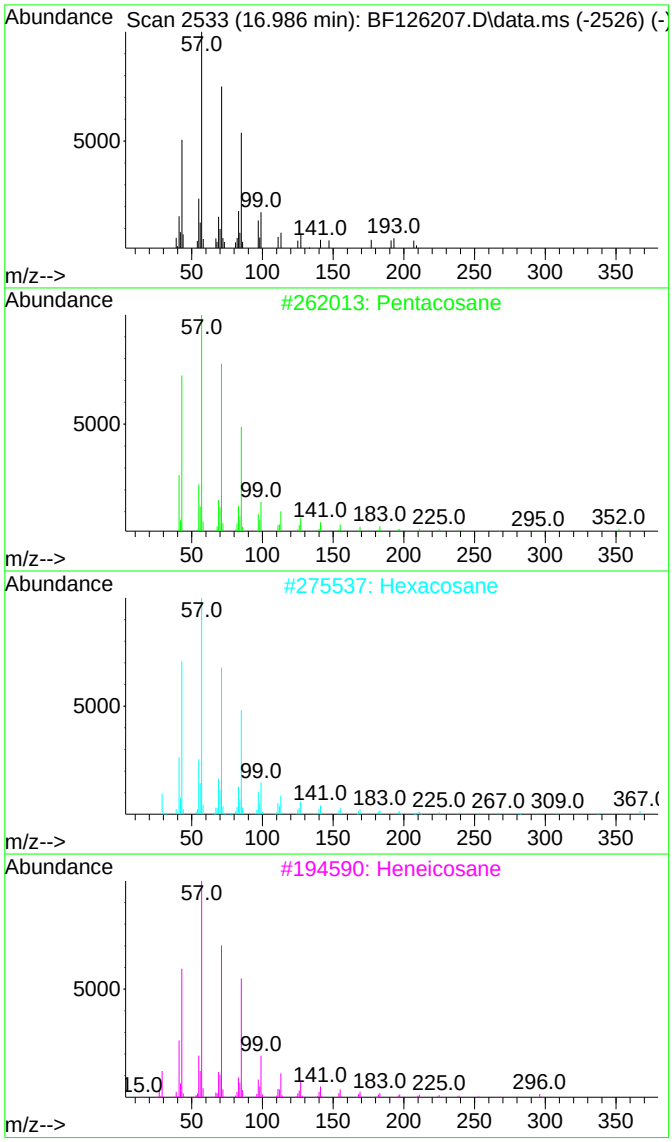
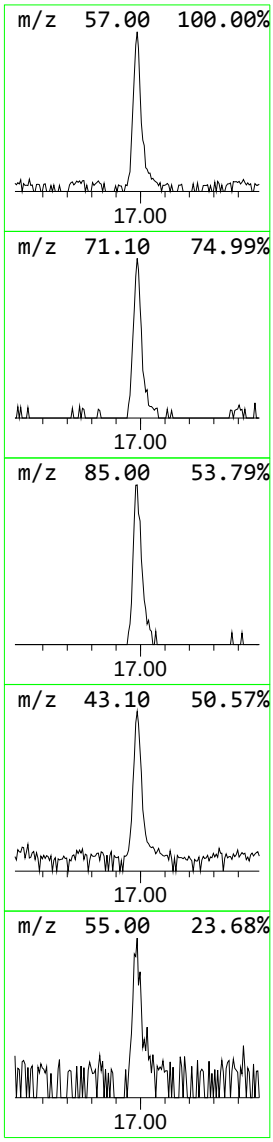
Peak Number 4 Pentacosane Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.986 | 2.05 ng | 102536 | Perylene-d12 | 15.410 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pentacosane | 352 | C25H52 | 000629-99-2 | 83 |
| 2 | Hexacosane | 366 | C26H54 | 000630-01-3 | 83 |
| 3 | Heneicosane | 296 | C21H44 | 000629-94-7 | 83 |
| 4 | Tetratetracontane | 619 | C44H90 | 007098-22-8 | 83 |
| 5 | Methoxyacetic acid, 2-tetradecyl... | 286 | C17H34O3 | 1000282-04-8 | 80 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121621\
Data File : BF126207.D
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Operator : JU/CG
Sample : PB141409BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PB141409BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

| | | | | | --Internal Standard--- | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Eicosane | 15.468 | 3.0 | ng | 149049 | 6 | 15.410 | 999321 | 20.0 |
| Octacosane, 2-m... | 15.898 | 2.9 | ng | 144601 | 6 | 15.410 | 999321 | 20.0 |
| Heptadecane | 16.398 | 2.7 | ng | 135465 | 6 | 15.410 | 999321 | 20.0 |
| Pentacosane | 16.986 | 2.0 | ng | 102536 | 6 | 15.410 | 999321 | 20.0 |